AFRL-OSR-VA-TR-2015-0088

Theoretical Study of Novel Nanostructured Materials for Lithium-Ion Batteries

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CENTRO DE INVESTIGACION EN MATERIALES AVANZADOS, S.C.

03/16/2015
Final Report

Air Force Research Laboratory
AF Office Of Scientific Research (AFOSR)/ IOS
Arlington, Virginia 22203
Air Force Materiel Command

REPORT DOCUMENTATION PAGE

Form Approved
OMB No. 0704-0188

1. REPORT DATE *(DD-MM-YYYY)*
21-04-2015

2. REPORT TYPE
Final Performance

3. DATES COVERED *(From - To)*
01-04-2013 to 30-09-2014

4. TITLE AND SUBTITLE
Theoretical Study of SiGeLi Clusters for Design of Novel Nanostructured Materials to Be Utilized as Anodes for Lithium-ion Batteries

5a. CONTRACT NUMBER

5b. GRANT NUMBER
FA9550-13-1-0175

5c. PROGRAM ELEMENT NUMBER

6. AUTHOR(S)
Mario Sanchez-Vazquez

5d. PROJECT NUMBER

5e. TASK NUMBER

5f. WORK UNIT NUMBER

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)
CENTRO DE INVESTIGACION EN MATERIALES AVANZADOS, S.C.
AV. MIGUEL DE CERVANTES NO. 120
CHIHUAHUA, 31109 MX

8. PERFORMING ORGANIZATION REPORT NUMBER

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)
AF Office of Scientific Research
875 N. Randolph St. Room 3112
Arlington, VA 22203

10. SPONSOR/MONITOR'S ACRONYM(S)
AFOSR

11. SPONSOR/MONITOR'S REPORT NUMBER(S)

12. DISTRIBUTION/AVAILABILITY STATEMENT
A DISTRIBUTION UNLIMITED: PB Public Release

13. SUPPLEMENTARY NOTES

14. ABSTRACT
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15. SUBJECT TERMS
lithium batteries

16. SECURITY CLASSIFICATION OF:			**17. LIMITATION OF ABSTRACT**	**18. NUMBER OF PAGES**	**19a. NAME OF RESPONSIBLE PERSON**
a. REPORT	**b. ABSTRACT**	**c. THIS PAGE**			Mario Sanchez-Vazquez
U	U	U	UU		**19b. TELEPHONE NUMBER** *(Include area code)* 52-8111-560812

Standard Form 298 (Rev. 8/98)
Prescribed by ANSI Std. Z39.18

Theoretical study of $Si_xGe_yLi_z^-$ (x=4-10, y=1-10, z=0-10) clusters for designing of novel nanostructured materials to be utilized as anodes for Lithium-ion batteries

Final Report

Nancy Perez-Peralta and Mario Sanchez-Vazquez

Abstract

In order to find out if silicon nanostructured materials resist lithium cations insertion and extraction under the presence of germanium atoms, we have explored theoretically the potential energy surface of Si_6Ge^-, $Si_6GeLi_5^-$, $Si_6GeLi_7^-$, $Si_6GeLi_{10}^-$, $Si_6Ge_2^-$, $Si_6Ge_2Li_5^-$, and $Si_{10}Ge_{10}Li_{10}^-$ clusters. This study was performed using the Kick Coalescence method coupled to Gaussian 09 program, and re-optimization all structures with the B3LYP/def2-TZVPP method. Our results confirm that incorporating germanium atoms to silicon clusters improves and prevents fragmentation.

Introduction

Rechargeable Li-ion batteries are the most promising energy storage devices for hybrid, plug-in hybrid electric, and all-electric vehicles. Lithium is an ideal material for batteries: it is the lightest metal in addition to having a high electric potential. Charging a Li-ion battery usually means moving lithium cations from cathode into anode. There is an increasing interest in developing rechargeable lithium batteries with higher energy capacity and longer cycle life for applications in portable electronic devices and electric vehicles. Currently, the graphite anode is the most commercially used due to its good capacity (372 mA h g^{-1}) together with its rate capability and long life. Silicon has recently become very popular as a potential anode material for lithium batteries because it has a low discharge potential and the highest known theoretical charge capacity (which could be 10x that of ghaphite).[1-4] However, silicon anodes have limited applications because of the large volume change upon lithium cations insertion or extraction. Silicon nanowires have been shown to be promising as high-performance lithium battery anodes because the can accommodate large strains derived from lithium charging or discharging.[3]

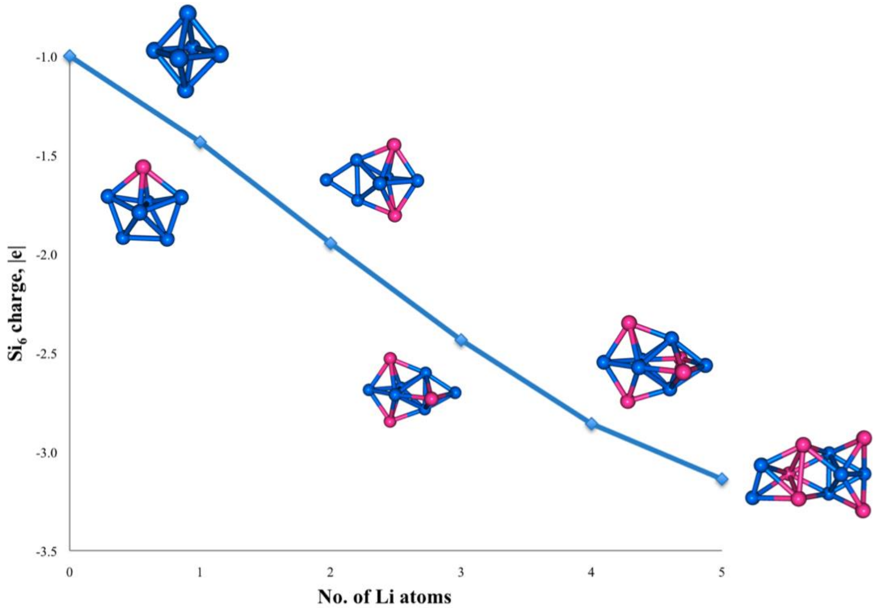


Figure 1. Si_6 skeleton charges for every global minimum structure vs. the number of lithium atoms are plotted. As one can see, the addition of five lithium atoms splits the Si_6 skeleton into two fragments: a S_4 kernel and a two-silicon fragment.

Very recently, an *ab initio* study on the lithiation of the Si_4^- cluster was reported. Results of this study revealed that the maximum formal charge transfer from alkali metals to Si_4 system is four and that the Si_4^- tetrahedral kernel is a robust building block.[5] However, a study on the lithiation of the Si_6^- shows that lithium cations are able to split the silicon skeleton into two fragments: the S_4 kernel and a two-silicon fragment (see Figure 1). This result actually gives an explanation to the large volume change of silicon anodes upon lithium cations insertion. The latter study suggests that even though the tetrahedral Si_4^{4-} structure is resistant, any material designed upon it will be broken up by lithium cations.[6] Song et al. have recently reported that Si/Ge double-layered nanotubes (Si/Ge DLNT) are promising materials as anodes for Li-ion batteries. Compared to silicon nanotubes, Si/Ge DLNT improve both cyclability and rate capability.[7] It is apparent from the last results that germanium atoms play a key role in the silicon structure stabilization upon lithium cations insertion and extraction. Therefore, we have proposed to investigate both qualitatively and quantitative germanium effects on silicon skeletons.

Computational details

In order to find out if silicon nanostructured materials resist lithium cations insertion and extraction under the presence of germanium atoms, we have been studying theoretically the lithiation process of the $Si_xGe_y^-$ (x=4-10, y=1-10) clusters. At the moment, we have explored the potential energy surfaces of the $Si_xGe_yLi_z^-$ (x=6, y=1-2, z=0-10) clusters throughout global minimum search techniques, i.e., Kick Coalescence method.[8]

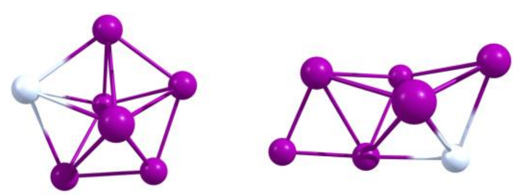
In order to find the global minimum structure of any cluster, a comprehensive scanning on the corresponding potential energy surface has been performed using the Kick Coalescence

method. Kick Coalescence (KC) method, is particularly powerful given that it combines the accuracy of *ab initio* and DFT approximations with a very fast scanning of any potential energy surface; in addition, it is unbiased. In this method, a very large population of structures that are generated randomly is subjected to a coalescence procedure with all atoms being pushed gradually to the molecular center of mass to avoid fragmented structures. Subsequently, these structures are optimized to the nearest local minimum using an electronic structure package. Currently, the KC method is coupled to Gaussian 09; but it can be easily coupled to any software that calculates electronic structure of atoms and molecules. At this stage, a low level of theory is required in order to get a fast scanning. In previous works on silicon clusters, reliable results have been got using the combination of the hybrid functional B3LYP with the 3-21G basis set. This optimization process was followed by a reoptimization and frequency calculation at a higher level of theory; B3LYP/def2-TZVPP has been used in the present research.

Results

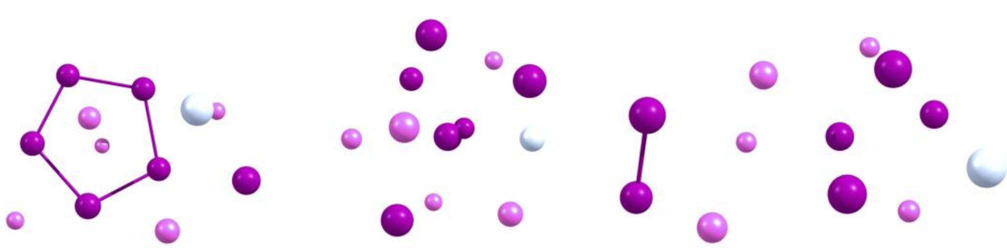
At the moment, we have explored the potential energy surface of Si_6Ge^-, $Si_6GeLi_5^-$, $Si_6GeLi_7^-$, $Si_6GeLi_{10}^-$, $Si_6Ge_2^-$, $Si_6Ge_2Li_5^-$, and $Si_6Ge_{10}Li_{10}^-$ clusters. Low-lying isomers structures are depicted in Figure 2. As is can be seen, Si_6 skeleton is distorted in order to accommodate the Ge atom in Si_6Ge^-. The global minimum structure, **1A**, corresponds to a planar five-member ring shaped by four Si atoms and one Ge atom, with other two Ge atoms located above and below the ring. The second most stable isomer, **1B**, is 14.0 kcal·mol^{-1} less stable than **1A**.

Si_6Ge^-



1A, Si_6Ge^- ΔE = 0.0 kcal·mol^{-1} — **1B**, Si_6Ge^- ΔE = 14.0 kcal·mol^{-1}

$Si_6GeLi_5^-$



2A, $Si_6GeLi_5^-$ ΔE = 0.0 kcal·mol^{-1} — **2B**, $Si_6GeLi_5^-$ ΔE = 0.6 kcal·mol^{-1} — **2C**, $Si_6GeLi_5^-$ ΔE = 0.9 kcal·mol^{-1}

$Si_6GeLi_7^-$

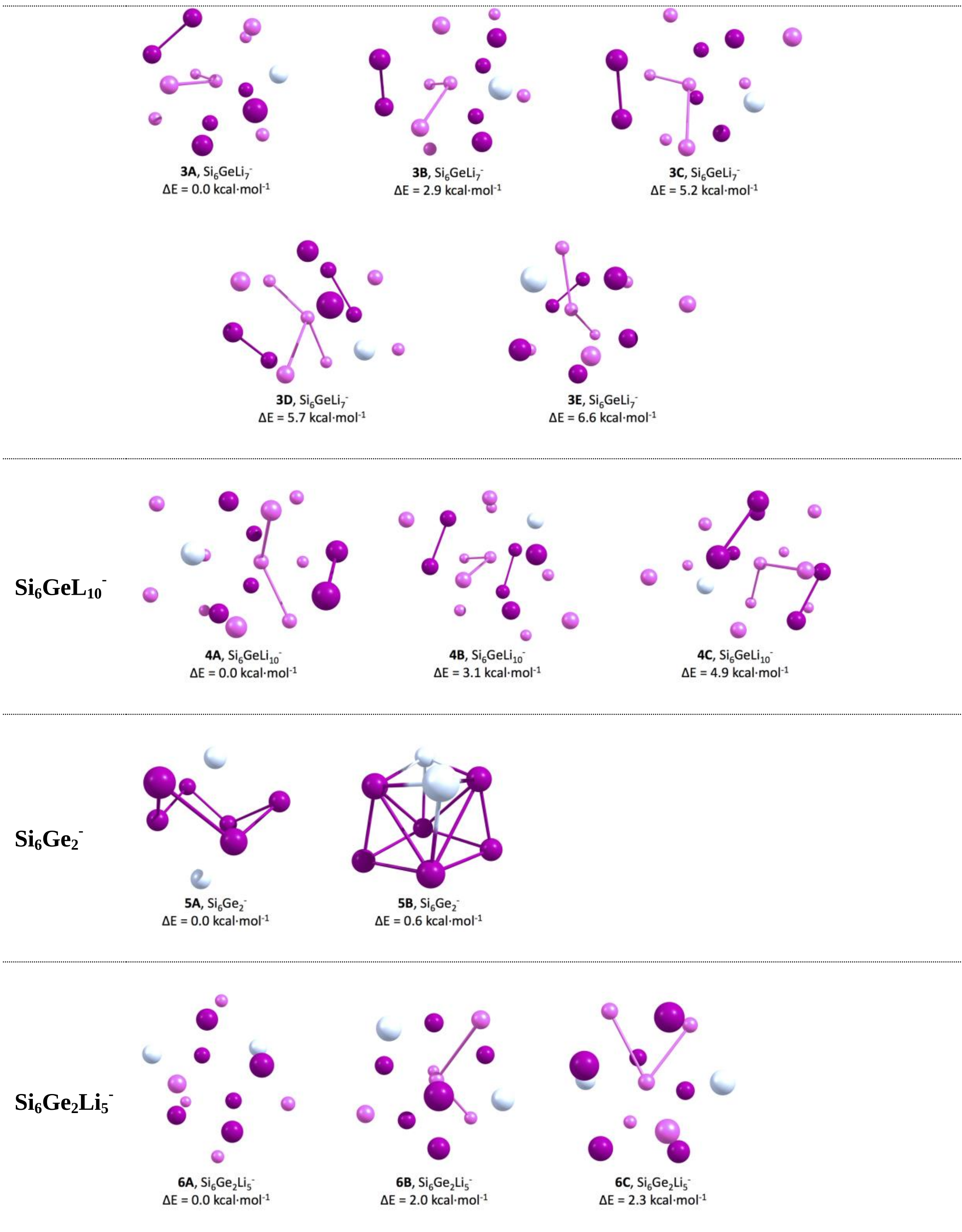


Figure 2. Low-lying isomers of Si_6Ge^-, $Si_6GeLi_5^-$, $Si_6GeLi_7^-$, $Si_6GeLi_{10}^-$, $Si_6Ge_2^-$, and $Si_6Ge_2Li_5^-$ clusters calculated at the B3LYP/def2-TZVPP level. Si atoms are represented by dark-pink spheres, Ge by white spheres, and Li by light-pink spheres.

Given that Si_6^- is fragmented when five Li atoms are added, we decided to explore the insertion of five Li atoms into the Si_6Ge^- cluster. The global minimum for $Si_6GeLi_5^-$ corresponds to structure **2A**, which consists of a planar five-member Si ring surrounded by the remaining Si atoms, one Ge atom and five Li atoms. It is noticeable that Si_6 skeleton is not longer fragmented by the five Li atoms. However, there are a number of isomers lying in the range of 0 – 1 kcal·mol^{-1}, where the Si_6 skeleton is actually fragmented. These results suggest that even though one Ge atom helps to prevent Si fragmentation, it is not enough. In order to corroborate our conclusion, we decided to explore $Si_6GeLi_7^-$, and $Si_6GeLi_{10}^-$. As it can be seen in Figure 2, silicon-germanium skeleton is fragmented by Li atoms in both cases.

Subsequently, we decided to explore the effect of the addition of two Ge atoms to Si_6^- cluster. Only two low-lying isomers were found: **5A** and **5B**. Isomer **5A** resembles chair conformation of cyclohexane with the Ge atoms located above and below the Si ring. The second most stable isomer, **5B**, can be seen as two Si tetrahedrons bridged by the Ge atoms. The relative energy between both isomers is only 0.6 kcal·mol^{-1}. When five Li atoms are added to the $Si_6Ge_2^-$ cluster, the resulting minimum structure corresponds to **6A**. This structure can be seen as a silicon aggregate surrounded by Ge and Li atoms. However, the second most stable isomer, **6B**, is a silicon-fragmented structure. Nonetheless, it is noticeable, that the difference in energy is 2.0 kcal·mol^{-1} now. This result suggests that incrementing the Ge atoms into the silicon cluster actually prevents its fragmentation. Because of that, we decided to study the biggest system proposed, $Si_{10}Ge_{10}Li_{10}^-$.

After exploring the potential energy surface of $Si_{10}Ge_{10}Li_{10}^-$, the structure depicted in Figure 3 was found to be the global minimum. This structure accommodates two distorted silicon tetrahedra connected by a silicon atom, surrounded by other three silicon atoms as well as the germanium fragment divided into two skeletons that also corresponds to two distorted tetrahedra. The lithium atoms are accommodated around the Si-Ge skeleton. There is no fragmentation due to lithium atoms in this structure. The last result confirms that actually germanium atoms prevent fragmentation of the silicon structure, as well as the tetrahedral skeleton of silicon atoms can be used as building-block fragment that stabilizes these materials.

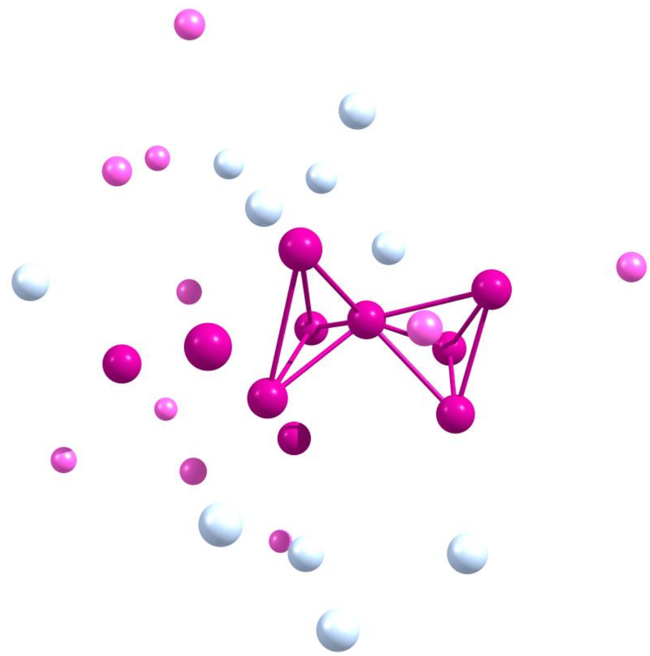


Figure 3. Global minimum structure of $Si_{10}Ge_{10}Li_{10}^{-}$ (**7A**).

The future work consists of studying materials based on the tetrahedral skeleton of silicon atoms, surrounded by tetrahedral fragments of germanium atoms. Such a material should resist fragmentation and be adequate to be used as anode in Li-ion batteries.

Finally, the xyz Cartesian coordinates are described below in order to provide better detail of the studies in this work. These Cartesian coordinates can be displayed in programs such as Mercury, ArgusLab, etc, or some other program that supports this type of coordinates.

Cartesian coordinates

1A

14	-0.308418000	2.114693000	-0.000392000
14	2.136519000	-1.302871000	0.000211000
14	-0.308292000	-2.114602000	0.000156000
14	2.136153000	1.302904000	-0.000109000
14	0.346930000	0.000601000	1.581198000
14	0.346973000	-0.000395000	-1.581184000
32	-1.903066000	-0.000145000	0.000052000

1B

14	0.923207000	-1.121609000	0.000373000
14	3.284098000	-0.788374000	-0.000194000
14	1.920375000	1.422610000	-0.000149000
14	-0.183384000	0.900110000	1.408206000

14	-0.183205000	0.900655000	-1.407640000
14	-2.162027000	1.439057000	0.000007000
32	-1.574590000	-1.204196000	-0.000264000

2A

14	-0.855176000	-0.809783000	-1.950081000
14	-0.614792000	0.020476000	2.143840000
14	1.290649000	-1.585002000	1.518766000
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3	2.276060000	1.014034000	1.802286000

2B

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3	2.177464000	-1.212471000	1.762285000
3	-3.588246000	2.787280000	-0.227890000
3	-1.793569000	0.122072000	1.815605000
3	1.236513000	2.207029000	-1.006320000

2C

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3	2.459019000	-1.955538000	-1.273827000

3A

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3B

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3C

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3E

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4A

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32	-2.025480000	-1.102978000	-0.239796000

5B

14	1.154075000	2.327987000	-0.000229000
14	-0.697501000	-1.670797000	0.000236000
14	0.652044000	-1.340103000	2.031767000
14	-0.329155000	0.950059000	-1.452032000
14	0.654051000	-1.341499000	-2.030159000
14	-0.330245000	0.950978000	1.451235000
32	-2.410068000	0.172668000	-0.000641000
32	1.927388000	-0.118691000	0.000283000

6A

14	0.624761000	-0.733039000	-1.647412000
14	-0.748956000	2.136761000	1.162102000
14	0.168358000	-1.709867000	1.135875000
14	-0.872951000	1.349944000	-1.475552000
14	1.430981000	1.806176000	0.024208000
14	-1.602874000	-0.112929000	1.953131000
32	-1.837916000	-0.977746000	-0.589241000
32	2.362850000	-0.588581000	0.258485000
3	1.521328000	1.550585000	-2.499168000
3	0.944768000	0.486135000	2.222179000
3	-0.199935000	3.688783000	-0.756870000
3	-0.270870000	-3.056037000	-0.938908000
3	-2.924741000	1.265141000	0.123191000

6B

14	1.200013000	-0.160550000	2.322537000
14	-2.048754000	1.467690000	0.312541000
14	1.308928000	1.134272000	-1.703933000
14	0.261642000	-1.307364000	-1.782288000
14	-1.245593000	-0.348351000	2.027744000
14	-0.103133000	2.783334000	-0.495122000
32	-1.989356000	-1.120434000	-0.466004000
32	2.189759000	-0.713156000	0.018039000
3	-1.292561000	0.907152000	-2.150048000
3	2.162476000	1.814923000	0.684776000
3	0.169748000	-2.234277000	0.799537000
3	0.026322000	0.311185000	0.127338000
3	-0.278099000	2.103840000	2.136454000

6C

14	-1.079847000	0.675598000	2.100388000

14	-1.068367000	-1.860034000	-1.443054000
14	1.081525000	-0.678713000	2.098375000
14	0.995137000	-2.164854000	-0.128486000
14	1.066977000	1.861941000	-1.441993000
14	-0.994268000	2.164954000	-0.125471000
32	-2.395838000	-0.105942000	-0.132672000
32	2.395595000	0.106367000	-0.133167000
3	1.216387000	1.952095000	1.320722000
3	-1.216879000	-1.953397000	1.318127000
3	-1.241219000	0.724007000	-2.327962000
3	1.239178000	-0.721563000	-2.329105000
3	-0.000277000	-0.000509000	-0.091705000

7A

14	-0.115042000	3.096381000	-1.225232000
14	-0.649485000	-3.094037000	1.792278000
14	1.017738000	-1.266001000	-1.268817000
14	-2.193980000	-2.290292000	0.092447000
14	-1.077238000	1.692851000	0.540410000
14	-0.421502000	-0.632928000	0.562040000
14	0.347253000	0.806245000	2.509680000
14	-0.383818000	-3.524855000	-1.008768000
14	-1.242096000	2.324515000	3.472236000
14	-2.860892000	0.834607000	-3.771554000
32	2.178435000	3.830716000	-1.477292000
32	-4.642127000	-1.724956000	-0.103207000
32	5.360294000	-0.348154000	0.670459000
32	-3.576706000	-0.158653000	-1.915350000
32	6.035191000	0.543553000	-1.327734000
32	-3.144496000	1.523499000	1.983169000
32	2.947394000	-1.075178000	0.347284000
32	4.109931000	-1.091408000	2.817559000
32	2.796800000	1.021802000	1.955362000
32	-4.686008000	-0.326328000	2.178105000
3	1.873680000	-3.543860000	0.374346000
3	-2.691937000	2.697858000	-1.691818000
3	-0.316956000	0.637134000	-2.685120000
3	2.161279000	1.072247000	-0.986518000
3	-1.961386000	-0.887968000	2.981444000
3	1.385545000	3.121609000	1.072669000
3	4.234286000	2.632518000	0.223602000
3	0.375433000	4.649317000	-3.145985000
3	1.414987000	-1.709448000	2.691336000
3	-5.218972000	0.156502000	-4.406860000

References

(1) Li, H.; Huang, X.; Chen, L.; Wu, Z.; Liang, Y. *Electrochem. Solid-State Lett.* **1999**, *2*, 547.
(2) Holzapfel, M.; Buqa, H.; Hardwick, L. J.; Hahn, M.; Wursig, A.; Scheifele, W.; Novak, P.; Kotz, R.; Veit, C.; Petrat, F. M. *Electrochimica Acta* **2006**, *52*, 973.
(3) Chan, C. K.; Peng, H. L.; Liu, G.; McIlwrath, K.; Zhang, X. F.; Huggins, R. A.; Cui, Y. *Nature Nanotechnology* **2008**, *3*, 31.
(4) Key, B.; Bhattacharyya, R.; Morcrette, M.; Seznec, V.; Tarascon, J. M.; Grey, C. P. *Journal of the American Chemical Society* **2009**, *131*, 9239.
(5) Perez-Peralta, N.; Boldyrev, A. I. *Journal of Physical Chemistry A* **2011**, *115*, 11551.
(6) Perez-Peralta, N.; Boldyrev, A. I. *Unpublished manuscript*.
(7) Song, T.; Cheng, H.; Choi, H.; Lee, J.-H.; Han, H.; Lee, D. H.; Yoo, D. S.; Kwon, M.-S.; Choi, J.-M.; Doo, S. G.; Chang, H.; Xiao, J.; Huang, Y.; Park, W. I.; Chung, Y.-C.; Kim, H.; Rogers, J. A.; Paik, U. *Acs Nano* **2012**, *6*, 303.
(8) Sergeeva, A. P.; Averkiev, B. B.; Zhai, H.-J.; Boldyrev, A. I.; S, W. L. *Journal of Chemical Physics* **2011**, *134*, 224304.

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Theoretical study of SixGeyLiz- (x=4-10, y=1-10, z=0-10) clusters for designing of novel nanostructured materials to be utilized as anodes for Lithium-ion batteries

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AFOSR assigned control number. It must begin with "FA9550" or "F49620" or "FA2386".

FA9550-13-1-0175

Principal Investigator Name

The full name of the principal investigator on the grant or contract.

Mario Sanchez-Vazquez

Program Manager

The AFOSR Program Manager currently assigned to the award

Mr. James Fillerup

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Abstract

In order to find out if silicon nanostructured materials resist lithium cations insertion and extraction under the presence of germanium atoms, we have explored theoretically the potential energy surface of Si6Ge-, Si6GeLi5-, Si6GeLi7-, Si6GeLi10-, Si6Ge2-, Si6Ge2Li5-, and Si10Ge10Li10- clusters. This study was performed using the Kick Coalescence method coupled to Gaussian 09 program, and re-optimization all structures with the B3LYP/def2-TZVPP method. Our results confirm that incorporating germanium atoms to silicon clusters improves and prevents fragmentation.

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